Solutions of the Fokker–Planck equation for a Morse isospectral potential

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Abstract

This work explores the relation between the Fokker–Planck equation and the Schrödinger equation in order to study solutions for the first one. The starting point is the study of the Schrödinger equation for a Morse potential. The next step is to determine the isospectral potential by using the formalism of supersymmetric quantum mechanics. Quantum isospectral potentials have the same energy spectrum of the original Morse potential, but the wavefunctions are different. Therefore, the transition probability that results from the Fokker–Planck equation for the Morse isospectral potential is different from that obtained for the original potential. This approach generates an entire class of new results.

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1. Introduction

A small enough macroscopic particle immersed in a liquid shows a random type of move because of the collisions with neighbor particles or by interacting with some external system. As well as the particle in a liquid, there are several other similar phenomena, for example, the chain fluctuations that exist in an electrical resistance [1]. This phenomenon is known as the Brownian move and clearly shows the statistical fluctuations in a system.

The Fokker–Planck equation was first applied to problems related to the Brownian move, in order to handle originated fluctuations of several small disorders, which made the molecules collide with particles around them and created an unexpected path when the position of the particles changed. Thus, it was impossible to determine the accurate position of the particles, but it was possible to determine the probability of finding them in a certain region.

In the literature, there are several examples of applications of the Fokker–Planck equation in areas of physics, such as studies of the tensor of molecular attrition for rotational and translational moves of Brownian particles near to surfaces [2] and analysis of the behavior of

great or weighed ions in fluids submitted to the electric field [3], among others. This shows the versatility and the importance of the applications of the Fokker–Planck equation, including from chemical–physical and biology up to uses in fields like physics of the solid state and astronomy.

This work aims to present a study of the statistical fluctuations that occur in some systems. Specifically, the Fokker–Planck equation related to the Schrödinger equation for the Morse potential and for the Morse isospectral potential is studied.

The Morse potential has been used to describe phenomena, such as hydrogen bonds in physical models for DNA [4, 5]. The isospectral potential obtained from the harmonic oscillator has also been used for this purpose [6]. Several works have been dedicated to the study of the Morse potential from the quantum point of view [7–9]. On the other hand, few works about this potential from the classical point of view are relevant [10, 11].

The construction of the isospectral potential by using the factorization operator was first made for the harmonic oscillator [12]. After this original work, several isospectral potentials are introduced in the literature (see, for instance, [13, 14]). A suggestion to use the isospectral potentials associated with the Fokker–Planck equation was presented in [15]. In the case studied in this work, isospectral potentials have the same energy spectrum of the original Morse potential, but the wavefunctions are different [16]. A recent approach is the use of this kind of potentials in the biological context to describe, for example, impurities in the structures of the microtubules, which can be represented by proteins or the discontinuity in the arrangement of tubulin molecules [17, 18].

In section 2 there is a short introduction of the Fokker–Planck equation and its relation with the Schrödinger equation. The original Morse potential is studied in section 3 by using the mathematical formalism of the supersymmetric quantum mechanics. In section 4 the Fokker–Planck equation for the Morse potential is presented. The isospectral potential to the Morse potential is shown in section 5. As illustration of the obtained results, numerical examples are indicated in section 6. Finally, in section 7 are the conclusions.

2. The Fokker–Planck equation

The Fokker–Planck equation can be obtained from the Langevin equation [19] and provides the temporal evolution of the probability distribution $P(x, t)$:

$$\frac{\partial}{\partial t} P(x, t) = -\frac{\partial}{\partial x}[f(x)P(x, t)] + \frac{\Gamma}{2}\frac{\partial^2}{\partial x^2} P(x, t), \qquad (1)$$

where $f(x)$ is the function related to a potential $V(x)$ and Γ is a constant.

The solution of the Fokker–Planck equation can be obtained through the method of variable separation, in which the probability distribution is the form

$$P(x, t) = \sum_{l=0}^{\infty} a_l \phi_l(x)\, e^{-t|\Lambda_l|}. \qquad (2)$$

The formalism of the supersymmetric quantum mechanics [20] can be used in the resolution of different equations of the Schrödinger-type equation. In this direction it is possible to write the Fokker–Planck equation (1) in terms of an equation of this type; for this, an operator $\hat{\omega}$ is used:

$$\frac{\partial}{\partial t} P(x, t) = \hat{\omega} P(x, t), \qquad (3)$$

and the functions $\phi_l(x)$ are considered, which are given by the expression $\phi_l(x) = \psi_l(x)\psi_0(x)$. $\psi_l(x)$ are the set of eigenfunctions of a Hermitian operator $\widehat{\kappa}$ defined by

$$\widehat{\kappa}\psi_l(x) = \frac{\widehat{\omega}[\psi_0(x)\psi_l(x)]}{\psi_0(x)}. \tag{4}$$

When the definitions above are used, it is possible to write the Fokker–Planck equation associated with the Schrödinger equation [19]:

$$\widehat{\kappa}\psi = -\frac{1}{2}\left\{\frac{\partial f}{\partial x} + \frac{1}{\Gamma}f^2\right\}\psi + \frac{\Gamma}{2}\frac{\partial^2 \psi}{\partial x^2}. \tag{5}$$

Thus, the solution of the Fokker–Planck equation is given by

$$P(x,t) = \psi_0(x)\sum_{l=0}^{\infty}a_l\psi_l(x)\,\mathrm{e}^{-t|\Lambda_l|}, \tag{6}$$

where $\psi_l(x)$ are the eigenfunctions and Λ_l are the eigenvalues of equation (5). The values for the coefficients a_l are given by [21]

$$a_l = \int_{-\infty}^{+\infty}P(x,0)\frac{\psi_l}{\psi_0}\,\mathrm{d}x = \frac{\psi_l(0)}{\psi_0(0)}. \tag{7}$$

The approach adopted here to analyze the Fokker–Planck equation can be found in some books (see, for example, [19]), and a recent revision on the subject is made in [22].

3. Supersymmetry

The supersymmetry appeared in the context of the physics of particles and fields and allowed relating bosons and fermions. The application of this concept in quantum mechanics gave rise to the so-called supersymmetric quantum mechanics, which was introduced in 1981 by Witten [23]. A quite interesting application is its use to obtain solutions of the Schrödinger equation [20].

In general lines, the formalism involves the factorization of a Hamiltonian for the so-called bosonic operators:

$$a^{\pm} = \mp\frac{d}{\mathrm{d}x} + W(x), \tag{8}$$

where $W(x)$ is called the superpotential.

By using the ideas of the supersymmetrical formalism, the Hamiltonian H_+ can be factorized in terms of bosonic operators:

$$H_+ = -\frac{\hbar^2}{2m}\frac{d^2}{\mathrm{d}x^2} + V(x) = a^+a^- + E_{+,0}. \tag{9}$$

The development of the equality above, when the definition of bosonic operators (8) is used, results in

$$W^2 - W' + E_{+,0} = V(x), \tag{10}$$

where $E_{+,0}$ is the eigenvalue of the ground state and $V(x)$ is the studied potential. For simplicity, $\hbar = 2m = 1$ is adopted. This equation is known as the Riccati equation, whose solution provides the superpotential $W(x)$. When the superpotential is determined, it is possible to obtain the wavefunction for ground state, by applying the bosonic operator a^- in the wavefunction for ground state ($a^-\psi_{+,0} = 0$):

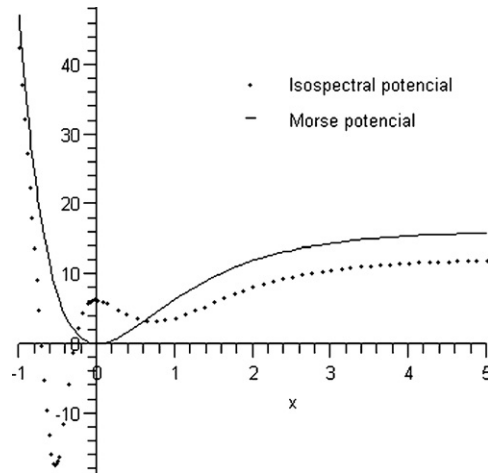$$\psi_{+,0} \propto \mathrm{e}^{-\int W(x)\,\mathrm{d}x}. \tag{11}$$

Figure 1. Graph of the Morse potential (continuous line) and its isospectral potential (dotted line) versus position *x*.

The algebraic structure of the supersymmetry allows the building of a hierarchy of Hamiltonians, in which the members are related among themselves [20]. Through the relation between eigenvalues and eigenfunctions of the hierarchy members, it is possible to determine the eigenfunctions and the eigenvalues associated with the original Hamiltonian H_+. This can be made for all potentials that are exactly soluble, in particular for the Morse potential [8].

The one-dimensional Morse potential is given by

$$Vm(x) = D(1 - e^{-ax})^2, \tag{12}$$

where D and a are constants. The continuous line in figure 1 shows the function $Vm(x)$ versus the position x with $D = 16$ and $a = 1$.

When we substitute the potential given for (12) in the Schrödinger equation and change the variable $y = ax$, we have

$$-\frac{d^2}{dy^2}\psi_n(y) + \lambda^2(1 - e^{-y})^2\psi_n(y) = \varepsilon_n\psi_n(y), \tag{13}$$

where $\lambda^2 = \frac{2mD}{a^2\hbar^2}$ and $\varepsilon_n = \frac{2mE_n}{a^2\hbar^2}$. In this case, the superpotential is written as [8, 16]

$$W(y) = \lambda(1 - e^{-y}) - \tfrac{1}{2}. \tag{14}$$

The form of the superpotential can be directly verified when we substitute the expression (14) in the Riccati equation (10), using $V(x)$ instead of the Morse potential (12).

The solution of equation (13) [8, 9, 16] is

$$\psi_n(y) = N\exp\left[-y\left(\lambda - n - \tfrac{1}{2}\right)\right]\exp(-\lambda e^{-y})L_n^{(2\lambda-2n-1)}(2\lambda e^{-y}) \tag{15}$$

$$\varepsilon_n = 2\lambda\left(n + \tfrac{1}{2}\right) - \left(n + \tfrac{1}{2}\right)^2, \qquad n = 0, 1, \ldots\left[\lambda - \tfrac{1}{2}\right], \tag{16}$$

where $L_n^\beta(x)$ is the associated Laguerre polynomial [24] and N is the normalization constant.

4. The Fokker–Planck equation for the Morse potential

Equation (5) shows that the operator $-\widehat{\kappa}$ can be identified as a Hamiltonian operator. In that equation, the function $f(x)$ is related to an effective potential. In this case, this effective potential is the Morse potential and can be written as

$$\frac{1}{2}\left\{\frac{[f(x)]^2}{\Gamma} + \frac{\partial f(x)}{\partial x}\right\} = V_{\text{eff}}(x) = D(1 - \mathrm{e}^{-ax})^2 + \frac{a^2\Gamma}{8} - \frac{a\sqrt{2D\Gamma}}{2}. \quad (17)$$

The solution of the differential equation above gives the explicit form of $f(x)$, i.e.

$$f(x) = \frac{a\Gamma}{2} - \beta + \beta\,\mathrm{e}^{-ax}, \quad (18)$$

where $\beta = \sqrt{2D\Gamma}$.

Thus, the expression of the force, given by equation (18), leads to the effective potential (17), i.e. to the Morse potential. Substituting equation (18) into equation (5), we obtain the following differential equation:

$$\frac{\Gamma}{2}\frac{d^2}{dx^2}\psi(x) - \frac{1}{2}\left\{-a\beta\,\mathrm{e}^{-ax} + \frac{1}{\Gamma}\left[\left(\frac{a\Gamma}{2} - \beta\right) + \beta\,\mathrm{e}^{-ax}\right]^2\right\}\psi(x) = \Lambda_n\psi(x). \quad (19)$$

The eigenvalues Λ_n of equation (19) can be determined by a direct comparison of this equation with the Schrödinger equation. The relation between these two equations is found by a direct way, when we relate $\Gamma \to \frac{\hbar^2}{m}$. From the obtained relation, the eigenvalues of equation (6) are established in terms of the eigenvalues given in equation (16). Explicitly, we have

$$\Lambda_n = \frac{a^2\Gamma n^2}{2} + \frac{a^2\Gamma n}{2} - a\beta n. \quad (20)$$

5. Isospectral potential to Morse potential

Another kind of potential analyzed here is the isospectral one, which is obtained from the original Morse potential. By using the method of factorization in supersymmetric quantum mechanics it is possible to find potentials with different functional forms. These potentials have the same energy spectrum as that of the original potential; for this reason they are called isospectrals [13].

To obtain the isospectral potential, a new superpotential $g(y)$ is defined as a more general form of the original superpotential:

$$g(y) = W(y) + \varphi(y), \quad (21)$$

where $W(y)$ is the superpotential related to the original Morse potential (14) and $\varphi(y)$ is a function to be determined by imposing the equality between the supersymmetric partner of the Hamiltonian written in terms of $W(y)$ and written by the new superpotential $g(y)$. The adopted proceeding follows the same way that is indicated in [12, 13] and can be applied to any well-defined potential. In the case studied here, the general form found for $g(y)$ is [16]

$$g(y) = \lambda(1 - \mathrm{e}^{-y}) - \frac{1}{2} + \varphi(y), \quad (22)$$

$$\varphi(y) = \frac{\exp[-y(2\lambda - 1) - 2\lambda\,\mathrm{e}^{-y}]}{\Delta + \int_0^y \exp[-\xi(2\lambda - 1) - 2\lambda\,\mathrm{e}^{-\xi}]\,d\xi}, \quad (23)$$
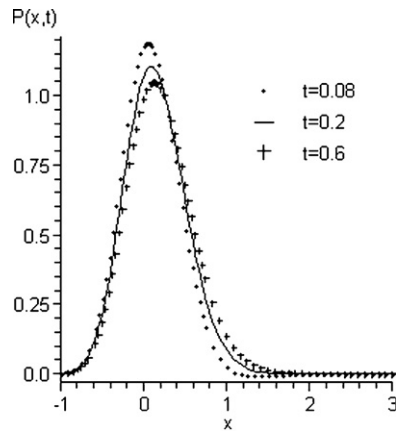
where Δ is an arbitrary constant.

Figure 2. Graph of the distribution of probability $P(x, t)$ versus x for Morse potential for different values of time.

When the value of the superpotential $g(y)$ is known, it is possible to determine the new potential, whose functional form is different from the original Morse potential. In this case, the potential is written as

$$Viso = \lambda^2(1 - e^{-y})^2 - \lambda + \tfrac{1}{4} - 2\varphi'(y). \tag{24}$$

The form of potential (24) depends on the adopted parameters. As an example, the dotted line in figure 1 shows the curve of the isospectral potential *Viso* versus the position x (remember that $y = ax$) to $D = 16$, $a = 1$, and $\Delta = 1.2 \times 10^{-5}$. It is observed that, in the choice of the parameters, the potential has two asymmetrical minimums, which contrasts with the original Morse potential presented in the same figure.

Once the eigenfunctions and the eigenvalues for the original Morse potential are known, the eigenfunctions given by the potential (24) can be determined through the relation

$$\Psi_{+,n} = A^+ a^- \psi_{+,n}, \tag{25}$$

where $A^+ = -\frac{d}{dy} + g(y)$ and $a^- = \frac{d}{dy} + W(y)$. This construction can be made for all energy levels, except for the ground state, that is obtained by the relation

$$A^- \Psi_{+,0} = 0. \tag{26}$$

In the studied case, the eigenfunction for the ground state is

$$\Psi_{+,0} = \exp\left[-\lambda(y + e^{-y}) + \frac{y}{2} - \int_0^y \varphi(\rho)\, d\rho \right]. \tag{27}$$

6. Numerical results

The functions $P(x, t)$, given by equation (6), correspond to the obtained probability distributions and they are different depending on the studied potential. The first studied potential is the Morse one. In equations (15) and (20) there are written, respectively, the wavefunctions and eigenvalues, which can be used to build the probability $P(x, t)$ by using equation (6).

The curves presented in figure 2 show $P(x, t)$ versus x for the original Morse potential in different times. In this numerical example, the parameters used for the potential have been
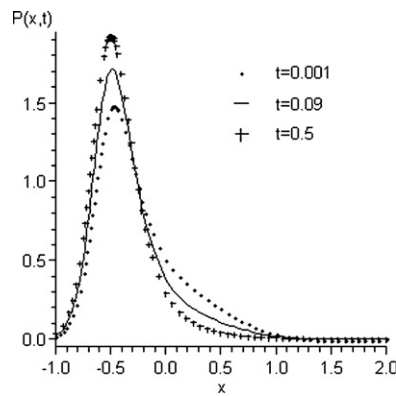
Figure 3. Graphic of the distributions of probability $P(x, t)$ versus x for isospectral potential to Morse potential for different values of time.
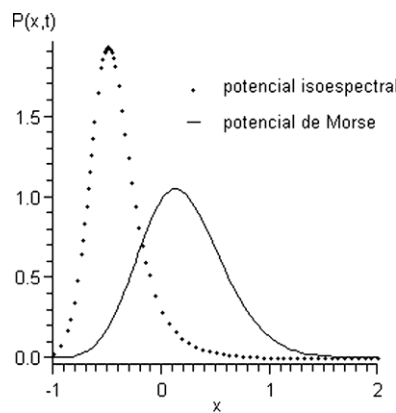

Figure 4. Graphic of the distributions of probability $P(x, t)$ versus x for isospectral potential to Morse potential and for the original Morse potential for large values of time.

$D = 16$, $a = 1$ and $\Gamma = 2$. With these parameters all the numerical constants of the problem are determined.

From figure 2 it can be observed that for small values of time the probability of finding a certain particle in a position x near the origin is large. As the time increases, this probability decreases. Another observation for this example is that for values of time higher than 0.6, the system can be considered stationary, which means that the curves for higher values of time are practically coincidental. This happens because the term dependent on the time in equation (6) becomes worthless, and contributes less and less while the time increases.

The second potential studied is the isospectral potential to Morse potential, which has the same energy spectrum (20) as that of the original Morse potential. However, the calculated wavefunctions in the two cases are different. The eigenfunctions of the isospectral potential are given by equation (25), except the ground state, in which the wavefunction is given by equation (27).

The curves shown in figure 3 exemplify the variation of the probability $P(x, t)$ with the position x for different values of time obtained in equation (6). In this case, the parameters used are the same ones that were indicated in the definition of the potential plotted in figure 1, i.e. $D = 16$, $a = 1$, and $\Delta = 1.2 \times 10^{-5}$.

From figure 3 it is observed that for small values of time, the probability distribution presents a deformation in the region that corresponds to the second minimum of energy of the studied potential (figure 1). For large values of time this deformation becomes small. This is an indication that the influence of second minimum diminishes. It is observed that for values higher of time than 0.5, the system can be considered stationary, which means that the term dependent on the time in equation (6) can be despised for time higher than that one. Graphically, it is observed that the curves with $t > 0.5$ are coincidental.

For a comparison, in figure 4 the distributions of probability for the two studied potentials in the stationary condition (large values of time) are plotted. We observe that the profiles of the curves are quite different.

The numerical results presented in this section are obtained from the expansion form of $P(x, t)$, equation (6); four terms are used in that expression. In this approximation the numerical errors are less than 10^{-6} for each point in the curves shown in figures 2–4.

7. Conclusions

The Fokker–Planck equation is analyzed for the Morse and its isospectral potential. Exact solutions can be determined in both cases by using the relationship between the Schrödinger equation and the Fokker–Planck equation.

From the analysis of figure 2, it is possible to observe that the values of the distribution of the probability in a position near to the origin are always high. For values of time higher than 0.6, the presented probability distributions are practically coincidental; in other words, the system gets in a stationary condition.

By observing figure 3, one notices that the probability distribution has a maximum near to the value $x = -0.5$. For values of time higher than 0.5 the system can be considered stationary. It is noticed, as expected, that the probability of finding the system in the region that corresponds to the second minimum of the potential (shallower well) is smaller than the probability of finding it in the region corresponding to the first minimum, which is deeper. The increase of the time results in a narrower curve of the probability distribution and an increase of the probability distributions near to the deepest minimum.

Through the curves of probability distributions of the numerical examples (figures 2 and 3) different characteristics in the two studied cases can be observed, although the used parameters are similar—only the value of Δ was introduced for the isospectral potential. In both cases, for values of very high time, the systems go on a stationary probability (figure 4). However, the maximums of the curves of probability distribution are distinct in the two cases and the time evolution is diverse. By using the original Morse potential, the peak of the probability distributions diminishes and its width increases with time. On the other hand, when the isospectral potential is used, this effect is inverted, the probability distribution gets narrower and its maximum gets sharper.

Finally, it is important to point out that the isospectral potentials allow the building of a new class of problems with analytical/exact solutions of the Fokker–Planck equation. As it can be seen in the studied cases, the obtained results are distinct and can describe different physical situations.

Acknowledgments

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